ANDREW G. STACK

Group Leader, Geochemistry and Interfacial Sciences
Chemical Sciences Division
Oak Ridge National Laboratory
One Bethel Valley Road, P.O. Box 2008
Bldg. 4100, Rm. C346
Oak Ridge, TN 37831-6110
Phone: 865-574-8450, Fax: 865-574-4961
E-mail: stackag@ornl.gov

Professional Interests

Mineral surface chemistry, particularly nucleation, growth and dissolution. Geochemical reaction kinetics and mechanisms. Fate and transport of contaminants. Reactions in aqueous solutions and porous media.

Educational Background

Ph.D.	Geology	2002	University of Wyoming
M.S.	Geology	1999	University of Wyoming
B.S.	Geological Sciences: Geochemistry option	1997	Virginia Polytechnic Institute

Employment History

Group Leader, Geochemistry and Interfacial Sciences	Oak Ridge National Laboratory	2017-present
Senior R&D Staff	Oak Ridge National Laboratory	2014-present
Acting Division Director, Chemical Sciences	Oak Ridge National Laboratory	2017-2018
R&D Staff	Oak Ridge National Laboratory	2010-2013
Assistant Professor	Georgia Institute of Technology	2005-2010
Postgraduate Researcher	University of California, Davis	2002-2005
Graduate Research Assistant	University of Wyoming	1997-2002
Temporary Scientist Level I	Shepherd-Miller Inc.	1998
Graduate Teaching Assistant	University of Wyoming	1997
Hydrologist	U.S. Geological Survey	1994-1997

Honors & Awards

Outstanding Contributions to Geosciences Research Award (2014). U.S. DOE Basic Energy Sciences, Geosciences Program

Award for One of Top 14 Technical Presentations (out of > 300), Twelfth Annual Conference on Carbon Capture, Utilization & Sequestration. Pittsburgh, PA, May 13-16, (2013)

Finalist for Asylum Research AFM Image Contest (2014)

Profile featured at ORNL web-site (Part I, Part II), STEM Magazine (2015)

Profile featured in American Chemical Society's "College-To-Career" web-site (2014)

ORNL Incentivized Performance Awards (2018, 2016, 2015, 2014)

ORNL Supplemental Performance Awards (2013, 2012, 2011)

Mineralogical Society of America Undergraduate Award (1997)
U.S. Department of Interior On-the-Spot Award (1996)

Professional Activities and Service

Member, U.S. Department of Energy, Office of Science, Basic Energy Sciences Advisory Committee (2019-present)

Faculty Member, Bredesen Center for Interdisciplinary Research and Graduate Education, University Tennessee/Oak Ridge National Laboratory (2016-present)

Editorial Board Member, Geochemical Transactions (2013-present)

Member of ORNL Committees: Research Conflict of Interest Advisory Committee (2015-present); Technology Innovation Program Internal Review Committee (2018); Laboratory Directed Research and Development Internal Review Committee, "Next-Generation Techniques and Methods for Neutron Sciences" (2015-2017); Center for Accelerated Materials Modeling Advisory Committee (2015-2016)

Member of Adjunct Graduate Faculty, Wright State University (2013-2018)

Past Division Chair for the Geochemistry Division of the American Chemical Society (2015), Division Chair (2014), Program Chair (2013), Program-Chair Elect (2012), Awards Committee Member (2016-2018). Organizer of Geochemistry Division Programming at National American Chemical Society conferences (fall 2013, spring 2014)

Attended Alda-Kavli Leadership Program (2016), ORNL Developing Leadership Potential (2015), and ORNL Management Boot Camp (2013) courses

Organizer of symposia at Pacifichem (2015), semi-annual National American Chemical Society conferences (2×spring 2015, spring 2014, spring 2013, fall 2013), V. M. Goldschmidt Geochemical Society conferences (2×2015, 2012, 2×2010, 2009, 2007, 2005)

Member of the Proposal Study Council (2013) & Proposal Study Panel (2012) for the Molecular Foundry, a DOE Nanoscale Science Research Center

Served on U.S. National Science Foundation Geobiology and Low Temperature Aqueous Geochemistry review panels (2012, 2011, 2009)

Served on review panel for the U.S. Department of Energy Biological and Environmental Research Program triennial review of the Environmental Molecular Sciences Laboratory at Pacific Northwest National Laboratory (2011)

Member: *American Chemical Society, American Association for the Advancement of Science*

Community Workshop Participation

Panelist and Liaison to the Workshop Chair for the Experts' Workshop on Carbon Capture, Utilization and Storage for the Mission Innovation Challenge global initiative (2017)

Panelist for Department of Energy, Basic Energy Sciences workshop and contributor to factual document on Basic Research Needs for the Energy-Water Nexus (2017)

Panelist/Roundtable Expert for Department of Energy, Basic Energy Sciences workshops and contributor to report on Subsurface Technology and Engineering Research Program (SubTER) and a new Grand Challenge for Subsurface Science (2015)

Publications: h-index = 22. (DOIs are hyperlinks)

1. Wanhala, A. K.; Doughty, B. Bryantsev, V. S.; Wu, L.; Mahurin, S. M.; Jansone-Popova S.; Cheshire, M. C.; Navrotsky, A.; **Stack, A. G.** (2019) Adsorption Mechanism of Alkyl Hydroxamic Acid onto Bastnäsite: Fundamental Steps toward Rational Collector Design for Rare Earth Elements. *J. Coll. Int. Sci.* 553, 210-219, DOI: 10.1016/j.jcis.2019.06.025
2. Wang, H.-W.; Graham, T. R.; Mamontov, E.; Page, K.; **Stack, A. G**.; Pearce, C. I. (2019) Countercations Control Local Specific Bonding Interactions and Nucleation Mechanisms in Concentrated Water-in-Salt Solutions. *J. Phys. Chem. Lett.* 10, 3318-3325, DOI: 10.1021/acs.jpclett.9b01416
3. Deng, N.; **Stack, A. G.**; Weber, J.; Cao, B.; De Yoreo, J. J.; Hu, Y. (2019) Organic–mineral interfacial chemistry drives heterogeneous nucleation of Sr-rich $(Ba_x, Sr_{1-x})SO_4$ from undersaturated solution. *Proc. Nat'l. Acad. Sci.* DOI: 10.1073/pnas.1821065116
4. Semrouni, D.; Wang, W.-H.; Clark, S. B.; Pearce, C.; Page, K.; Schenter, G.; Wesolowski, D. J.; **Stack, A. G.**; Clark, A. E. (2019) Resolving local configurational contributions to X-ray and neutron radial distribution functions within solutions of concentrated electrolytes – a case study of concentrated NaOH. *Phys. Chem. Chem. Phys.* 21, 6828-6838 DOI: 10.1039/c8cp06802j
5. DiStefano, V. H.; McFarlane, J.; **Stack, A. G.**; Perfect, E.; Mildner, D. F. R.; Bleuel, M.; Chipera, S. J.; Littrell, K. C.; Cheshire, M. C.; Manz, K. E.; Anovitz, L. M. (2019) Solvent-pore interactions in the Eagle Ford shale formation. *Fuel*, 238, 298-311. DOI: 10.1016/j.fuel.2018.10.010
6. Bracco, J. N.; Lee, S. S.; Stubbs, J. E.; Eng, P. J.; Jinda, S.; Warren, D. M.; Kommu, A.; Fenter, P.; Kubicki, J. D.; **Stack, A. G.** (2019) Simultaneous Adsorption and Incorporation of Sr^{2+} at the Barite (001) – Water Interface. *J. Phys. Chem. C* 123, 1194-1207 DOI: 10.1021/acs.jpcc.8b08848
7. Graham, T. R.; Semrouni, D.; Mamontov, E.; Ramirez-Cuesta, A. J.; Page, K.; Clark, A. E.; Schenter, G. K.; Pearce, C. I.; **Stack, A. G.**; Wang, H-W. (2018) Coupled Multimodal Dynamics of Hydrogen-Containing Ion Networks in Water-Deficient, Sodium-Hydroxide-Aluminate Solutions. *J. Phys. Chem. B* 122, 12097-12106, DOI:10.1021/acs.jpcb.8b09375
8. Anovitz, L. M.; Zhang, X.; Soltis J.; Nakouzi, E.; Krzysko, A. J.; Chun, J.; Schenter, G. K.; Graham, T. R.; Rosso, K. M.; De Yoreo, J. J.; **Stack, A. G.**; Bleuel, M.; Gagnon, C.; Mildner, D. F. R.; Ilavsky, J.; Kuzmenko, I. (2018) Effects of Ionic Strength, Salt, and pH on Aggregation of Boehmite Nanocrystals: Tumbler Small-Angle Neutron and X-ray Scattering and Imaging Analysis. *Langmuir 34*, 15839-15853 DOI: 10.1021/acs.langmuir.8b00865

(FY19 start)

9. **Stack, A. G.**; Stubbs, J. E.; Srinivasan, S. G.; Roy, S.; Bryantsev, V. S.; Eng, P. J.; Custelcean, R.; Gordon, A. D.; Hexel, C. R. (2018) Mineral-Water Interface Structure of Xenotime (YPO_4) {100} *J. Phys. Chem. C* 122, 20232-20243 DOI:10.1021/acs.jpcc.8b04015
10. Weber, J.; Bracco, J. N.; Poplawsky, J. D.; Ievlev, A.; More, K. L.; Lorenz, M.; Bertagni, A. L.; Jindra, S. A.; Starchenko, V.; Higgins, S. R.; **Stack, A. G.** (2018) Unraveling the

Effects of Strontium Incorporation on Barite Growth – In-situ and Ex-situ Observations using Multi-Scale Chemical Imaging. *Cryst. Growth Des.* 18, 5521-5533 DOI: 10.1021/acs.cgd.8b00839

11. Wang, H.-W.; Vlcek, L.; Neuefeind, J.; Page, K.; Irle, S.; Simonson, J. S.; **Stack, A. G.** (2018) Decoding Oxyanion Aqueous Solvation Structure: A Potassium-Nitrate Example at Saturation. *J. Phys. Chem. B.* 122, 7584-7589 DOI: 10.1021/acs.jpcb.8b05895
12. Graham, T. R.; Dembowski, M.; Martinez-Baez, E.; Zhang, X.; Jaegers, N. R.; Hu, J.; Gruskiewicz, M. S.; Wang, H.-W.; **Stack, A. G.**; Bowden, M. E.; Delegard, C. H.; Schenter, G. K.; Clark, A. E.; Clark, S. B.; Felmy, A. R.; Rosso, K. M.; Pearce, C. I. (2018) In-Situ ^{27}Al NMR Spectroscopy of Aluminate in Sodium Hydroxide Solutions Above and Below Saturation with Respect to Gibbsite. *Inorg. Chem. 57,* 11864-11873 DOI: 10.1021/acs.inorgchem.8b00617
13. Cheshire, M. C.; Bish, D. L.; Cahil, J. F.; Kertesz, V.; **Stack, A. G.** (2018) Geochemical evidence for rare-earth element mobilization during kaolin diagenesis. *ACS Earth Space Chem.* 2*,* 503-520 DOI: 10.1021/acsearthspacechem.7b00124
14. Shen, Z.; Kerisit, S.; **Stack, A. G.**; Rosso, K. M. (2018) Free-Energy Landscape of the Dissolution of Gibbsite at High pH. *J. Phys. Chem. Lett.* 9, 1809-1814. DOI: 10.1021/acs.jpclett.8b00484
15. Cao, B.; **Stack, A. G.**; Steefel, C. I.; DePaolo, D. J.; Lammers, L. N.; Hu, Y. (2018) Investigating Calcite Growth Rates Using a Quartz Crystal Microbalance with Dissipation (QCM-D). *Geochim. Cosmochim. Acta 222*, 269-283. **DOI:** 10.1016/j.gca.2017.10.020
16. Bracco, J. N.; Lee, S. S.; Stubbs, J. E.; Eng, P. J.; Heberling, F.; Fenter, P.; **Stack, A. G.** (2017) Hydration Structure of the Barite (001)-Water Interface: Comparison of X-ray Reflectivity with Molecular Dynamics Simulations. *J. Phys. Chem. C 122*, 12236-12248 DOI: 10.1021/acs.jpcc.7b02943
17. De La Pierre, M.; Raiteri, A. G.; **Stack, A. G.**; Gale, J. D. (2017) Uncovering the atomistic mechanism for calcite step growth. *Angew. Chem. Int'l. Ed. 56*, 8464-8467 DOI: 10.1002/ange.201701701
18. Srinivasan, S. G.; Shivaramaiah, R.; Kent, P. R. C.; **Stack, A. G.**, Riman, R. E.; Anderko, A.; Navrotsky, A.; Bryantsev, V. S. (2017) A Comparative Study of Surface Energies and Water Adsorption on Ce-Bastnästite, La-Bastnästite, and Calcite via Density Functional Theory and Water Adsorption Calorimetry. *Phys. Chem. Chem. Phys. 19(11)*, 7820-7832. DOI: 10.1039/C7CP00811B
19. Wang, H.-W.; Daemen, L. L.; Cheshire, M. C.; Kidder, M. K.; **Stack, A. G.**; Allard, L. F.; Neuefeind, J.; Olds, D.; Liu, J.; Page, K. (2017) Synthesis and structure of synthetically pure and deuterated amorphous (basic) calcium carbonates. *Chem. Comm. 53, 2942-2945.* DOI: 10.1039/C6CC08848A
20. Cheshire, M. C.; **Stack, A. G.**; Carey, J. W.; Anovitz, L. M.; Prisk, T. R.; Ilavsky, J. (2017) Wellbore Cement Porosity Evolution in Response to Mineral Alteration During CO_2 Flooding. *Environ. Sci. Technol.* **51**, 692-698 DOI: 10.1021/acs.est.6b03290

21. **Stack, A. G.**; Borreguero, J. M.; Prisk, T. R.; Mamontov, E.; Wang, H.-W.; Vlcek, L.; Wesolowski, D. J. (2016) Precise determination of water exchanges on a mineral surface. *Phys. Chem. Chem. Phys.* **18**, 28817-28828 DOI: 10.1039/C6CP05836A
22. DiStefano, V. H.; McFarlane, J.; Anovitz, L. M.; **Stack, A. G.**; Gordon, A. D.; Littrell, K. C.; Chipera, S. J.; Hunt, R. D.; Lewis, S. A.; Hale, R. E.; Perfect, E. (2016) Extraction of organic compounds from representative shales and the effect on porosity. *J. Nat. Gas. Sci. Engr.*, 35, 646-660 DOI: 10.1016/j.jngse.2016.08.064
23. Godinho, J. R. A.; Gehrke, K. M.; **Stack, A. G.**; Lee, P. D. (2016) The dynamic nature of crystal growth in pores. *Sci. Rep.,* 6:33086 DOI: 10.1038/srep33086
24. Srinivasan, S. G.; Shivaramaiah, R.; Kent, P. R. C.; **Stack, A. G.**, Navrotsky, A.; Riman, R. E. Anderko, A.; Bryantsev, V. S. (2016) Crystal Structures, Surface Stability and Water Adsorption Energies of La-Bastnäsite via Density Functional Theory and Experimental Studies. *J. Phys. Chem. C*, 120, 2811-2829, DOI: 10.1021/acs.jpcc.6b04747
25. Dai, C.; **Stack, A. G.**; Koishi, A.; Fernandez-Martinez, A.; Lee, S. S.; Hu, Y. (2016) Heterogeneous Nucleation and Growth of Barium Sulfate at Organic-Water Interfaces: Interplay between Surface Hydrophobicity and Ba^{2+} Adsorption. *Langmuir* 32, 5277-5284 DOI: 10.1021/acs.langmuir.6b01036
26. Zachara, J.; Brantley, S.; Chorover, J.; Ewing, R.; Kerisit, S.; Liu, C.; Perfect, E.; Rother, G.; **Stack, A. G.** (2016) Internal Domains of Natural Porous Media Revealed: Critical Locations for Transport, Storage, and Chemical Reaction. *Environ. Sci. Technol.* 50, 2811-2829 DOI: 10.1021/acs.est.5b05015
27. **Stack, A. G.** (2015) Precipitation in Pores: A Geochemical Frontier. *Rev. Mineral. Geochem.* 80, 165-190 DOI: 10.2138/rmg.2015.80.05 (#1 or #2 most highly read RiMG article Sept., 2015 - Dec., 2015).
28. Godinho, J. R. A.; **Stack, A. G.** (2015) Growth kinetics and morphology of barite crystals derived from face-specific growth rates. *Cryst. Growth Des.* 15, 2064-2071 DOI: 10.1021/cg501507p
29. **Stack, A. G.**; Kent, P. R. C. (2015) Geochemical Reaction Mechanism Discovery from Molecular Simulation. *Environ. Chem.* 12, 20-32. DOI: 10.1071/EN14045
30. Hatzell, M. C.; Raju, M.; Watson, V. J.; **Stack, A. G.**; van Duin, A. C. T.; Logan, B. E. (2014) Effect of Strong Acid Functional Groups on Electrode Rise Potential in Capacitive Mixing by Double Layer Expansion. *Environ. Sci. Technol.* 48, 14041-14048. DOI: 10.1021/es5043782
31. Bracco, J. N.; **Stack, A. G.**; Higgins, S. R. (2014) Magnesite step growth rates as a function of the aqueous magnesium-to-carbonate ratio. *Cryst. Growth Des.* 14, 6033-6040. DOI: 10.1021/cg501203g
32. **Stack, A. G.**; Fernandez-Martinez, A.; Allard, L. F.; Bañuelos, J. L.; Rother, G.; Anovitz, L. M.; Cole, D. R.; Waychunas, G. A. (2014) Pore-Size-Dependent Calcium Carbonate Precipitation Controlled by Surface Chemistry. *Environ. Sci. Technol.* 48, 6177-6183. DOI: 10.1021/es405574a
33. **Stack, A. G.** (2014) Next generation models of carbonate mineral growth and dissolution. *Greenhouse Gases: Sci. Technol.* 4, 278-288. DOI: 10.1002/ghg.1400

34. Gazzè, S. A.; **Stack, A. G.**; Ragnarsdottir, K. V.; McMaster, T. J. (2014) Chlorite topography and dissolution of the interlayer studied with Atomic Force Microscopy. *Am. Mineral.* 99(1), 128-138. DOI: 10.2138/am.2014.4478
35. Qin, L.; Zhang, W.; Lu, J.; **Stack, A.G.**; Wang, L. (2013) Direct Imaging of Nanoscale Dissolution of Dicalcium Phosphate Dihydrate by an Organic Ligand: Concentration Matters. *Environ. Sci. Technol.* 47(23), 13365-13374. DOI: 10.1021/es402748t
36. Wang, H.-W.; Anovitz, L. M.; Burg, A.; Cole, D. R.; Allard, L. F.; Jackson, A. J.; **Stack, A. G**.; Rother, G. (2013) Multi-scale characterization of pore evolution in a combustion metamorphic complex, Hatrurim basin, Israel: Combining (ultra) small-angle neutron scattering and image analysis. *Geochim. Cosmochim. Acta*, 121, 339-362.
37. Bracco, J. N.; **Stack, A. G.**; Steefel, C. I. (2013) Upscaling Calcite Growth Rates From the Meso- to the Macro- Scale. *Environ. Sci. Technol.,* **47**, 7555-7562. DOI: 10.1021/es400687r
38. **Stack, A. G.**; Gale, J. D.; Raiteri, P. (2013) Virtual Probes of Mineral–Water Interfaces: The More Flops, the Better! *Elements*, 9, 211-216. DOI: 10.2113/gselements.9.3.211
39. Rother, G.; Ilton, E. S. Wallacher, D.; Hauß, T.; Schaef, H. T.; Qafoku, O.; Rosso, K. M.; Felmy, A. R.; Krukowski, E. G.; **Stack, A. G.**; Grimm, N.; Bodnar, R. J. (2013) CO_2 sorption to subsingle hydration layer montmorillonite clay studied by excess sorption and neutron diffraction measurements. *Environ. Sci. Technol.*, **47**, 205-211. DOI: 10.1021/es301382y
40. Bracco, J. N.; Grantham, M. C.; **Stack, A. G.** (2012) Calcite growth rates as a function of aqueous calcium-to-carbonate ratio, saturation index, and inhibitor concentration: Insights into the mechanism of reaction and poisoning by strontium. *Cryst. Growth Des.* **12**, 3540-3548. DOI: 10.1021/cg300350k
41. **Stack, A. G.**; Raiteri, P.; Gale, J. D. (2012) Accurate rates of the complex mechanisms for growth and dissolution of minerals using a combination of rare event theories. *J. Am. Chem. Soc.* **134**, 11-14. DOI: 10.1021/ja204714k
42. Zhang, W.; **Stack, A. G.**; Chen, Y. (2011) Interaction Force Measurement between *E. coli* Cells and Nanoparticles Immobilized Surfaces by Using AFM. *Colloids Surf. B*: *Biointerfaces* **82**, 316-324. DOI: 10.1016/j.colsurfb.2010.09.003
43. **Stack, A. G.**; Grantham, M. C. (2010) The growth rate of calcite steps as a function of aqueous calcium-to-carbonate ratio: independent attachment and detachment of calcium and carbonate ions. *Cryst. Growth Des.* **10**, 1409-1413. DOI: 10.1021/cg901395z
44. Zhang, M.; Burns, J. L.; DiChristina, T. J.; **Stack, A. G.** (2010) Attachment isotherms of *Shewanella oneidensis* to amorphous iron (oxy)(hydr)oxides. *Environ. Sci. Technol.* **44**, 1602-1609.
45. Wang, X.; Ingall, E.; Lai, B.; **Stack, A. G.** (2010) Self-assembled Monolayers as Templates for Heme Crystallization. *Cryst. Growth Des*. **10**, 798-805.
46. **Stack, A.G.** (2009) Molecular Dynamics Simulations of Solvation and Kink Site Formation at the {001} Barite-Water Interface. *J. Phys. Chem. C,* **113**, 2104-2110.
47. Zhang, M.; Dale, J. R.; DiChristina, T. J.; **Stack, A. G.** (2009) Dissolution morphology of iron (oxy)(hydr)oxides exposed to the dissimilatory iron reducing bacterium *Shewanella oneidensis* MR-1. *Geomicrobiol. J.,* **26**, 83-92.

48. Wigginton, N. S.; Rosso, K. M.; **Stack, A. G.**; Hochella, Jr. M. F. (2009) Long-Range Electron Transfer Across Cytochrome-Hematite (α-Fe_2O_3) Interfaces. *J. Phys. Chem. C,* **113**, 2096-2103.
49. **Stack, A.G.**; Rustad, J. R. (2007) Structure and Dynamics of Water on Aqueous Barium Ion and the {001} Barite Surface. *J. Phys. Chem. C*, 111, 16387-16391.
50. Rustad, J. R.; **Stack, A. G.** (2006) Molecular dynamics calculation of the activation volume for water exchange on Li^+. *J. Am. Chem. Soc.*, **128**, 14778-14779.
51. **Stack A. G.**, Rustad J. R., Casey W. H. (2005) Modeling water exchange on an aluminum polyoxocation. *J. Phys. Chem. B* (Letters) **109**, pp. 23771-23775.
52. **Stack A. G.**, Rustad J. R., Land T. A., De Yoreo J. J., Thomas T. N.& Casey W. H. (2004) The growth morphology of the {100} surface of KDP (Archerite) on the molecular scale. *J. Phys. Chem. B*. **108**, pp. 18284-18290.
53. **Stack A. G.**, Erni R., Browning N. D. & Casey W. H. (2004) Pyromorphite growth *in situ* on lead sulfides. *Envi. Sci. Technol*. **38**, pp. 5529-5534.
54. **Stack A. G.**, Eggleston C. M. & Engelhard M. H. (2004) Reaction of hydroquinone with hematite I: Electrochemical scanning tunneling microscopy and X-ray photoelectron spectroscopy. *J. Coll. Int. Sci.,* **274**, pp. 433-441.
55. **Stack A. G.**, Rosso K. M., Smith D. M. A. & Eggleston C. M. (2004) Reaction of hydroquinone with hematite II: Calculation of the electron transfer rate and comparison to the dissolution rate. *J. Coll. Int. Sci.,* **274**, pp. 442-450.
56. Eggleston C.M., **Stack A.G.**, Rosso K.M. & Bice A.M. (2004) Adatom Fe(III) on the hematite surface: Observation of a key reactive surface species. *Geochem. Trans.* **5**, 2, pp. 33-40.
57. Eggleston C. M., **Stack A. G.**, Rosso K. M., Higgins S. R., Bice A. M., Boese S. W., Pribyl R. D. & Nichols J. J. (2003) The structure of hematite (α -Fe_2O_3) (001) surfaces in aqueous media: Scanning tunneling microscopy and resonant tunneling calculations of coexisting O and Fe terminations. *Geochim. Cosmochim. Acta*. **67**, 5, pp. 985-1000.
58. **Stack A. G.**, Higgins S.R. & Eggleston C.M. (2003) Response to comment on "Point of zero charge of a corundum-water interface probed with optical second harmonic generation (SHG) and Atomic Force Microscopy (AFM): New approaches to oxide surface charge. *Geochim. Cosmochim. Acta*. **67**, 2, pp. 321-322
59. Higgins S. R., **Stack A. G.**, Knauss K. G., Eggleston C. M. & Jordan G. (2002) Probing molecular scale adsorption and dissolution-growth processes using nonlinear optical and scanning probe methods suitable for hydrothermal applications. In *Water-Rock Interactions, Ore Deposits, and Environmental Geochemistry: A Tribute to David A. Crerar*, Special Publication No. 7 (ed. R. Hellmann and S. A. Wood), pp. 111-128. The Geochemical Society.
60. **Stack A. G.**, Higgins S.R. & Eggleston C.M. (2001) Point of zero charge of a corundum-water interface probed with optical Second Harmonic Generation (SHG) and Atomic Force Microscopy (AFM): New approaches to oxide surface charge. *Geochim. Cosmochim. Acta* **65**, 18, pp. 3055-3063.

61. Higgins, S. R.; **Stack, A. G**.; Eggleston, C. M.; Afonso, M. D. S. (1998) Proton and ligand adsorption at silica-and alumina-water interfaces studied by optical second harmonic generation (SHG). *Mineral. Mag.*, **62**, 616-617.

Research Grants and Contracts

"Atomic- to Pore-Scale Geochemical Reaction Mechanisms." (ERKCC72) U.S. DOE, Office of Basic Energy Sciences, 10/1/2015-9/30/2018, $2,000k/yr. 6 person-months per year. Principal Investigator & Thrust 1 Leader (2015-present); Subtask 2 Leader (2012-2015); Subtask 1 Leader (2010-2012).

"IDREAM: Interfacial Dynamics in Radioactive Environments and Materials." (ERKCG08) U.S. DOE, Office of Basic Energy Sciences, 8/01/16 – 09/30/20, $3,000k/yr (ORNL portion $338k/yr). 3 person-months per year. ORNL Point of Contact and Leadership Team member (2016-present).

"Center for Nanoscale Control of Geologic CO_2, an Energy Frontier Research Center" (ERKCC67) U.S. DOE, Office of Basic Energy Sciences, 8/01/14 – 09/30/18, $3,200k/yr (ORNL portion $490k/yr). 3 person-months per year. ORNL Team Lead (2013-present),Team Member (2010-3013).

"Critical Materials Institute." (CEED500) U.S. DOE, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office. 6/29/2013 - present. 3 person-months per year. Project 1.1.12 Team Member (2018-present), Project 1.1.1 Team Leader (2015-2018); Project 1.1.1 Team Member (2013-2015).

"Reducing Environmental Impacts of Hydrofracturing by Subsurface Co-Precipitation of Barium and Radium." (LOIS6735) ORNL Laboratory Directed Research and Development. $388k/yr. 03/15/13 - 03/14/15. 2 person-months per year. Principal Investigator (2013-2015).

"Improving Chemical Separations through Understanding Weak Interactions" (ERKCC51) U.S. DOE, Office of Basic Energy Sciences, 8/1/12 – 7/31/15, $400k/yr. 2 person-months per year. Team Member (2012-2015).

"Testing Molecular Mechanisms for Growth and Dissolution Reactions on Calcite Surfaces" (Award #0643139) U.S. NSF, Earth Sciences Directorate, Geobiology and Low Temperature Aqueous Geochemistry program, 08/01/07 - 07/31/10, $219,385. Principal Investigator.

"Reaction mechanisms for barite dissolution and growth." (DE-FG02-07ER15901) U.S. DOE, Basic Energy Sciences Program, Geosciences Subprogram, 08/01/07 - 07/31/2009, $209,747. Principal Investigator.

"Characterization of Mineral Dust Aerosols to Improve Predictions of Their Impact on the Radiative Balance of the Atmosphere." U.S. NOAA, 04/01/07 - 03/31/10, $314,741. Co-Investigator.

Invited Talks and Symposia

1. "Calcite and Barite Mineral Precipitation in (Nano)Porous Media." *257th ACS National Meeting in Orlando, Florida*, March 31-April 4, 2019.

2. "Linking computational simulation with neutron diffraction to understand ion solvation structure and ion pairing in aqueous solutions. *255th ACS National Meeting in New Orleans, Louisiana,* March 18-22, 2018.
3. "Atomic-to pore-scale geochemistry: Effects of ion sorption and incorporation on mineral growth." *255th ACS National Meeting in New Orleans, Louisiana,* March 18-22, 2018.
4. "Insights into Geochemical Transformations Probed by Examining Solution and Solid Phase Structures Using Neutron Diffraction and Atomic-Scale Simulation." *U.S. DOE Basic Energy Sciences, Geosciences Program*, *Research PI Meeting*, August 7-8th, 2017.
5. "Quasi-Elastic Neutron Scattering Measured on a Mineral-Water Interface, Coupled to Process-Based Mineral Crystal Growth Models." *Oak Ridge National Laboratory, Joint Nanoscience and Neutron Scattering User Meeting*. August 1-2nd, 2017.
6. "Atomic- to Pore-Scale Probes of Mineral Reactivity in Subsurface Environments." *Brookhaven National Laboratory*, workshop on "*Synchrotron Techniques in Support of DOE's Subsurface R&D Effort.*" May 15-16th, 2017.
7. "Mineral Precipitation Reactions from the Atomic- to Pore-Scales." Departmental Seminar. *University of Delaware, Department of Geological Sciences.* May 4th, 2017.
8. "Atoms to pores concepts for mineral growth and precipitation." Session on "Geochemistry Division Medal: Symposium in Honor of Dr. Susan Brantley." *253rd ACS National Meeting in San Francisco, California,* April 2-6, 2017.
9. "Fast solvent exchange on a mineral-water interface coupled to process-based mineral precipitation models." Session on "Mineral-Water Interface Chemistry." *253rd ACS National Meeting in San Francisco, California,* April 2-6, 2017.
10. "Carbonation reactions and their effect on pore distributions in a cement exposed to CO_2 for 30^+ years." Session on "Pore-Scale Geochemical Processes & The Implications for CO_2 Geologic Storage." *253rd ACS National Meeting in San Francisco, California,* April 2-6, 2017. Also selected to be presented as a Sci-Mix poster.
11. "Towards a Fundamental Understanding of the Evolution of Porosity and Permeability During Mineral Nucleation and Growth" *American Geophysical Union Fall Meeting*, San Francisco, CA, December 12, 2016.
12. "Towards a fundamental understanding of the nucleation and growth of minerals in porous media." *U.S. DOE Basic Energy Sciences, Geosciences Program*, Research PI Meeting, August 15-16, 2016.
13. "Mineral Precipitation Reactions from the Atomic to Pore Scales" Departmental Seminar, *Institut des Sciences de la Terre, Centre National de la Recherche Scientifique/ Académie Grenoble*, Grenoble, France, Jan. 11, 2016.
14. "Mineral Precipitation Reactions from the Atomic- to Pore Scales." Departmental Colloquium, *Pennsylvania State University, Department of Geosciences*, Oct. 6, 2015.
15. "Precipitation in Pores" Keynote address in session "Pore Scale and Nano-Confined Geochemical Processes," *V. M. Goldschmidt Conference*, Aug., 20, 2015.

16. “Precipitation in Pores: A Geochemical Frontier” Short Course Lecture, *Reviews in Mineralogy and Geochemistry*, Volume 80, “Pore-Scale Geochemical Processes.” Aug. 15, 2015.
17. “Atomic- to Pore-Scale Understanding and Prediction of Mineral Precipitation.” Departmental seminar, *University of Houston, Dept. of Civil and Environ. Engineering*. Nov. 24, 2014.
18. “Atomic- to Pore-Scale Probes and Predictions of Mineral Reactivity.” *U.S. DOE Basic Energy Sciences, Geosciences Program*, Research PI Meeting, May 14-16, 2014.
19. “Atomic-scale to Mesoscale simulation of mineral growth and dissolution reactions.” *247th Meeting of the American Chemical Society*, Dallas, TX, March 16-20, 2014.
20. “Mechanisms and Rates of Reaction for Crystallization from the Atomic to Macroscopic Scales: Simulation, Theory and Experiment.” *Advanced Photon Source User Seminar Series*, Nov. 15, 2013.
21. “Upscaling Carbonate Mineral Growth Rates From the Nano- to Pore- Scales and Beyond: Current Progress and Future Directions.” *Twelfth Annual Conference on Carbon Capture, Utilization & Sequestration.* Pittsburgh, PA, May 13-16, 2013.
22. “Mechanisms and Rates of Reaction at Mineral-Water Interfaces from the Atomic to Pore Scales: Simulation, Theory and Experiment.” *Division Seminar, Chemical Sciences and Materials Sciences Divisions, ORNL*. April 17, 2013.
23. “Fast Water Exchange on a Mineral Surface Measured by Quasi-Elastic Neutron Scattering (QENS) and Classical Molecular Dynamics (MD).” Session on “Approaching the Surface: Interrogating Chemical Interactions at the Mineral-Water Interface.’ *245th Meeting of the American Chemical Society*, New Orleans, LA, April 7-11, 2013
24. “Nucleation and Growth of Minerals (Calcium Carbonate) in Porous Media” *U.S. DOE BES Geosciences Workshop* on “Reaction and Transport within Internal Domains of Porous Media” San Francisco, December 1-2, 2012.
25. “Calcite Growth from the Molecular Scale.” Session on Physicochemical constraints of the marine carbonate system: recent insights into the reactivity of carbonate minerals in aqueous solutions. *Goldschmidt 2012*, Montréal, Canada, June 24-29, 2012.
26. “Molecular level mechanisms of mineral growth and dissolution.” *Seminar for Geophysical Laboratory*. *Carnegie Institute*, Washington, D. C., January 9, 2012.
27. "Rates of mineral growth and dissolution reactions from molecular dynamics." Session on Large and Complex Atomistic Systems: Physics, Algorithms and Hardware. *Goldschmidt 2011*, Prague, Czech Republic, August 14-19, 2011.
28. “Interaction between iron respiring bacteria and iron (oxy)(hydr)oxides.” Departmental seminar at *Washington University at St. Louis*, Department of Earth and Planetary Sciences. September 17, 2009.
29. "Reactions controlling step movement during mineral dissolution and growth" Session on Molecular Computational Geochemistry for Water-Rock Interactions. *237th Meeting of the American Chemical Society*, Salt Lake City, March 22-26, 2009
30. “Applications of electrochemical scanning tunneling microscopy to adsorption and thin films in geochemical systems.” Session on Advanced Approaches to investigating

Adsorption at the solid–Water interface., *235th Meeting of the American Chemical Society*, New Orleans, LA, April 6-10, 2008

31. "Comparison of computational and experimental barite-water interface structures and kinetics." Session on Physical chemistry of environmental interfaces. *235th Meeting of the American Chemical Society*, New Orleans, LA, April 6-10, 2008
32. "Water structure on aqueous ions and barite-water interfaces." Division of Colloid and Surface Chemistry. *235th Meeting of the American Chemical Society*, New Orleans, LA, April 6-10, 2008.
33. "Prediction of ligand exchange and crystal growth kinetics using atomistic computational methods. Seminar. *William R. Wiley Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory*. Richland, WA, January 14th, 2008.
34. "Modeling water exchange on an aluminum polyoxocation." Seminar. *Chemical and Analytical Sciences Division, Oak Ridge National Laboratory*. Oak Ridge, TN, October 10th, 2005.

Advisees

Oak Ridge National Laboratory

Dr. Ke Yuan, ORNL post-doctoral researcher (2019-Present)
Dr. Alexander (Sandy) Brady, ORNL Post-Doctoral Researcher (2018-Present)
Mr. Nikhil Rampal, Research Advisor for Columbia Univ. Ph.D. Student (2018-Present)
Ms. Anna Wanhala, Bredesen Center Ph.D. Student (2015-Present)
Dr. Juliane Weber, Post-Doctoral Researcher (2017-2019) (Facility Manager, Univ. Arizona)
Dr. Min Liu, ORNL Post-Doctoral Researcher (2018-2019) (post-doc, LANL)
Dr. Hsiu-Wen Wang, Joint Institute for Neutron Scattering Researcher (2014-2018) (R&D Staff, ORNL)
Dr. Michael C. Cheshire, Post-Doctoral Researcher (2014-2016) (R&D Staff, ORNL)
Dr. José R. A. Godinho, Post-Doctoral Researcher (2013-2015) (Research Scientist, Helmholtz-Zentrum Dresden-Rossendorf)
Dr. Alexander D. Gordon, Post-Doctoral Researcher (2013-2014) (staff, Signature Science)

Georgia Institute of Technology

Dr. Jacquelyn N. Bracco, undergraduate & M.S. student (graduated spring 2012) (Ass't. Prof., CUNY)
Mr. Davis "Morgan" Warren, M.S. student (graduated spring 2011) (Private industry)
Ms. Cynthia M. Jackson, undergraduate student (graduated spring 2011) (graduate student, GSU)
Dr. Mengni Zhang, Ph.D. (Received departmental best paper award, 2009; graduated fall, 2010) (Environmental Scientist, NewFields, Inc.)
Dr. Xuefeng Wang, postdoctoral researcher (2008-2010) (Ph.D. Fellow, Seattle Children's Hospital)
Ms. Lindsay Wallace, non-thesis MS. (graduated spring 2010) (Environmental Scientist, NewFields, Inc.)

Academic Committee Service

Dissertation & Thesis Committee Membership

Nikhil Rampal, Ph.D., Columbia Univ. (expected 2022)
Samuel Evans, Ph.D. University of Tennessee, Knoxville (expected summer 2019)
Victoria DiStefano, Ph.D., University of Tennessee, Knoxville (summer, 2018)
Chong Dai, Ph.D., University of Houston (spring 2018)
Jacquelyn N. Bracco, Ph.D., Wright State University (fall 2015)
Dennis Lenaerts, M.S., Wright State University (spring 2013)

Department Committee Membership - Georgia Institute of Technology
Co-Chair, Graduate Student Acceptance Committee (2009/2010)
Graduate Student Acceptance Committee (2005-2009)
Undergraduate Curriculum Committee (2006/2007)
EAS Faculty Search Committee (2006/2007)
Multiple Graduate Student Thesis Committees (2005-2010)

Teaching Experience

Georgia Institute of Technology, School of Earth and Atmospheric Sciences

Semester	**Course**	**Title**	**Enrollment**
Spring, 2010	8803 (Grad)	Special Study: The Origin of Life	1
Fall, 2009	4110 (U.Grad)	Resources, Energy and the Environment	20
Fall, 2009	8803 (Grad)	Mineral Surface Geochemistry	10
Fall, 2009	4900 (U.Grad)	Special Study: C++ for Geochemists	3
Fall, 2008	4803/8803 (U.Grad/Grad)	Resources, Energy and the Environment	28
Spring, 2008	4803/8803 (U.Grad/Grad)	Water Quality Modeling	4
Fall, 2007	4803 (U.Grad)	Resources, Energy and the Environment	18
Spring, 2007	4803/8803 (U.Grad/Grad)	Water Quality Modeling	5
Fall, 2006	8803 (Grad)	Mineral Surface Geochemistry	9
Fall, 2005	4803/8803 (U.Grad/Grad)	Water Quality Modeling	5

University of Wyoming, Department of Geology and Geophysics

Semester	**Course**	**Title**	**Enrollment**
Summer, 2001 (U. Wyo. Wind River Reservation Extension)	GEOL/ASTR 1070	The Earth: Its Physical Environment	6

Teaching Assistantships:

1999-2002	U. Wyo.	The Earth: Its Physical Environment
1997	U. Wyo.	Physical Geology
1997	VPI	General Chemistry